

STRUCTURE AND BONDING

Chemistry has contents of Matter, Particles and Constituents. In studying bonding and Structure is to know what's holding the Constituents

The Constituents and Particles are many but we normally generalized. The Matter will be Solid, liquid, gas or plasma. The Constituents are held by chemical bond.

What is chemical bond

1. A chemical bond is a force of attraction that holds elements or atoms in a compound or element.

Example, Na — element

NaCl — Compound

2. A chemical bond is a link between two atoms or group of atoms when the forces acting between them are sufficient to lead to the formation of an aggregate (molecule) with sufficient stability to make it convenient for the chemist to consider it as an individual species.

FORCE is an attraction between two atoms or an element to form a bond and can not be seen with physical eyes.

The nature of a chemical bond holding atoms or ions has a major influence on the structure of the material.

FACTORS THAT DETERMINE THE STRUCTURES

1. The general formula of the substances or compound
2. The valencies of the elements present.
3. The relative size of the atoms or ions, species, particles.

Atoms consist of nucleus and electrons. The nucleus contains protons and neutrons, while the electrons arrange in shells, orbits or orbitals. Classical theory, Bohr theory, Quantum theory. Bohr theory stated that the particles of the nucleus which are the protons, neutrons and electrons must have a different giving number and when added together must have a neutral.

When you have two number of electrons, 3 number of protons and 1 number of neutron it is charged and the charge carries a positive sign because the number of protons are

much.

The OCTET RULE states that the maximum number to be carried in the first shell will not be more than two (2) while any other shell can carry maximum of eight and above. Example of orbitals

1. S
2. S, P
3. S, P, d
4. S, P, d, f

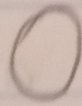
S = 2 electrons

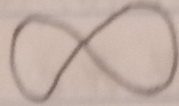
P = 6 electrons

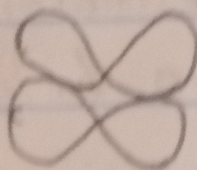
d = 10 electrons

f = 14 electrons

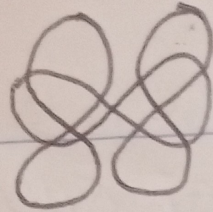
Each orbital is a mathematical representation geometrically the area where electrons can be found at a given point in time around the nucleus.

S — Shape  Spherical

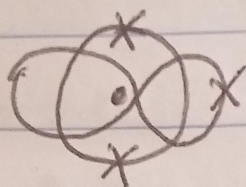
P — Principal  Dumb-bell

d — diffuse 

f — fundamental



CLASSICAL THEORY States that when the first shell that carries the two electrons which is the S-orbital, the other electrons form a shell that carries the P-orbital shapes.



If an atom have three electrons the structure will have two shells with the P-orbitals.

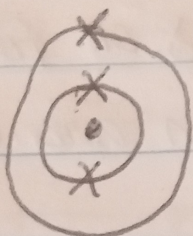
CHEMICAL BOND

Matter = Link = Force =

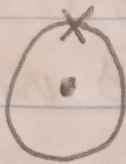
⇒ IONIC BONDING is when you generate ions and when the ions come together, and once the anion is brought close to a cation you experience a force of attraction. It has more Proton than electron.

All the Shell of an atoms which are not complete always look for something to react with. E.g Li, H, He, Be etc while the

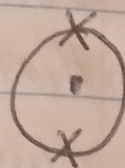
atoms that has a shell filled with complete electrons does not require anything to react with



Li



H

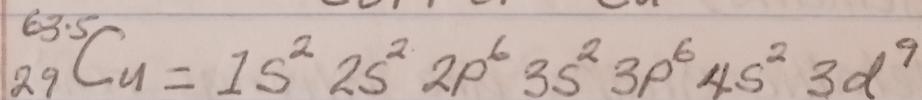


He

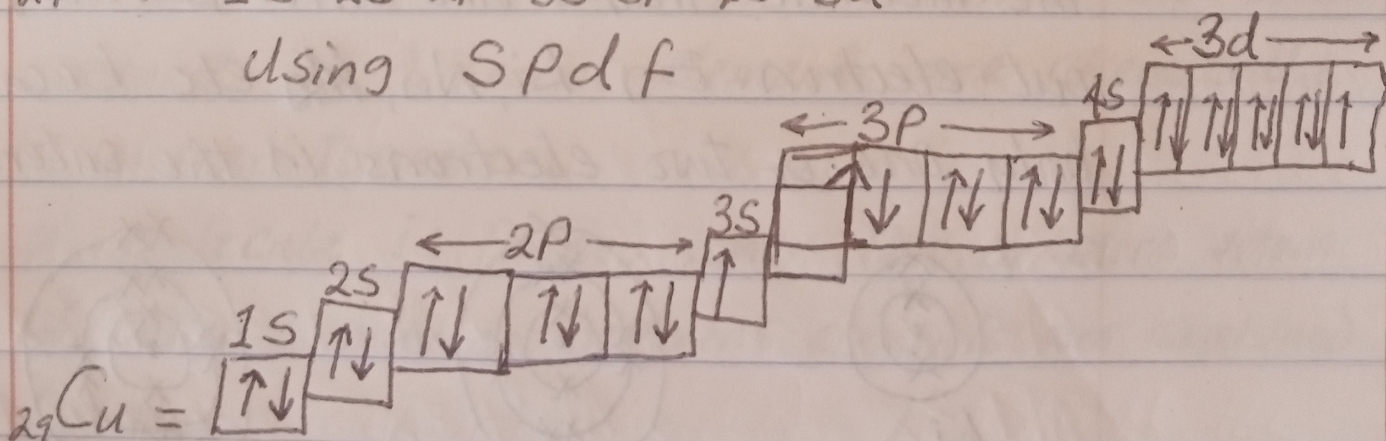
ASSIGNMENT

Write electronic configuration of an atom that is in group 29. [Atomic number 29]

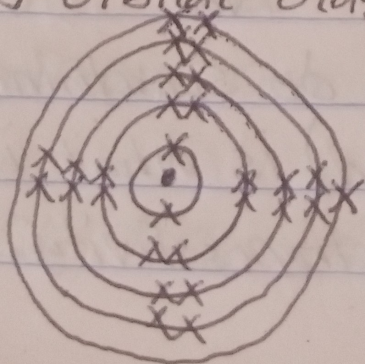
COPPER Cu



using S p d f



Using Orbital diagram.



2, 8, 8, 8, 3

Using Shell

If an atom has five shells and the other has three shells, the one with five shells is bigger. That is how atomic size is obtained. Ionic bonding is the bond or force of attraction that is created when anion and cation come close together.

General Chemical bonding

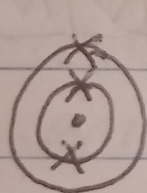
M ——— Metals

X ——— Non-metals

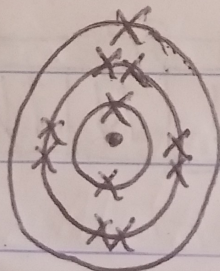
Group 1 and 2 are metals (column)

Group 4, 5, 6, 7, and 8 are non-metals (rows arrangements)

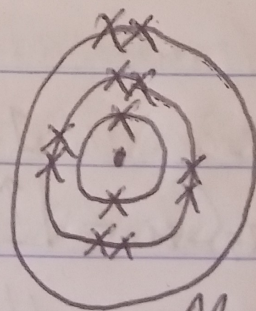
The metallic groups are always ready to give out electron. E.g Li, Na, ~~Mg~~ etc because it has only one or two electrons in the outermost shell.



Li



Na



Mg

The power to do something (i.e. either gain or loss electron) is what is called electronegativity or electropositivity.

The Cation is formed when electrons are given out to another and Cation is formed when electron is received from others.

$\text{Na} \longrightarrow \text{Na}^+ + \text{e}^-$ One electron released

$\text{Mg} \longrightarrow \text{Mg}^{2+} + 2\text{e}^-$ Two electrons released

$\text{Al} \longrightarrow \text{Al}^{3+} + 3\text{e}^-$ Three electrons released

The number of electrons given out must be shown or indicated at the top of the element.

The atom gains electron

~~$\text{N} + \text{e}^- \longrightarrow \text{N}^-$~~

~~$\text{O} + 2\text{e}^- \longrightarrow \text{O}^{2-}$~~

~~$\text{F} + 3\text{e}^- \longrightarrow \text{F}^{3-}$~~

A Compound is formed when atom of the same element or different elements are chemically combined together.

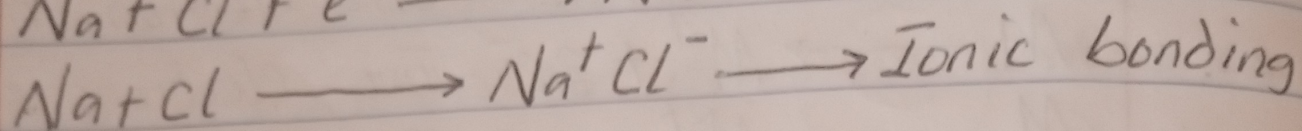
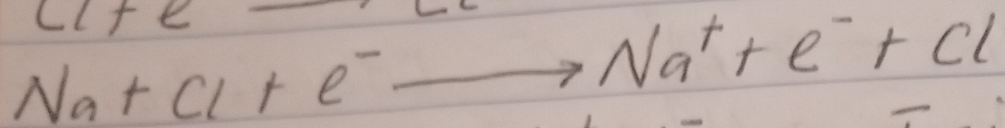
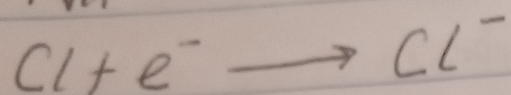
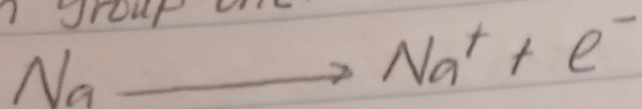
A Molecule is formed when two or more atom of either similar or different elements are combined together.

Electronegative $\longrightarrow$ HCl $\longrightarrow$ Non-Metal-Electropositive

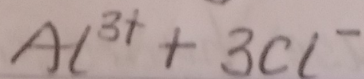
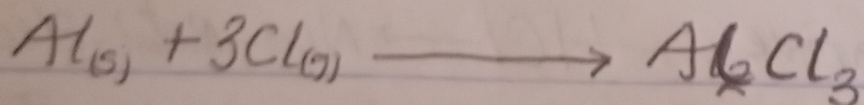
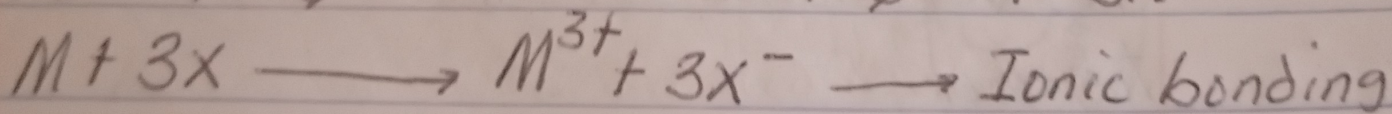
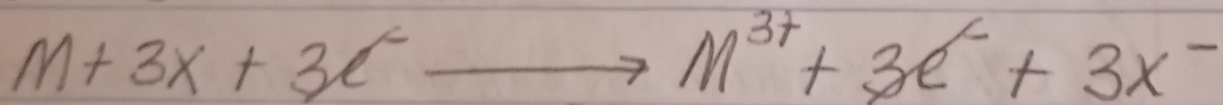
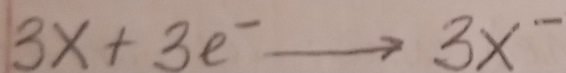
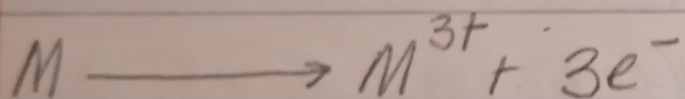
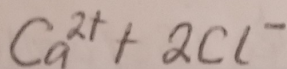
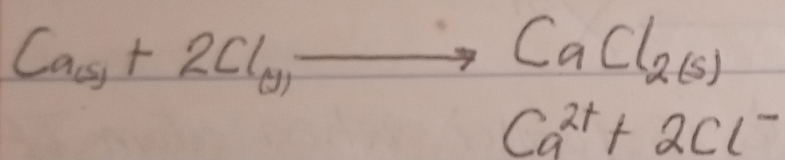
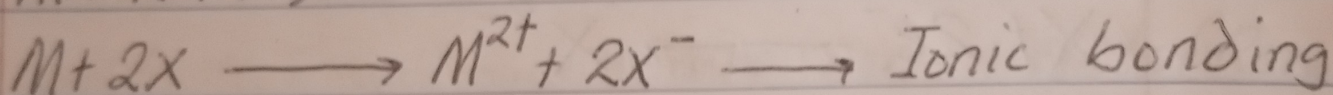
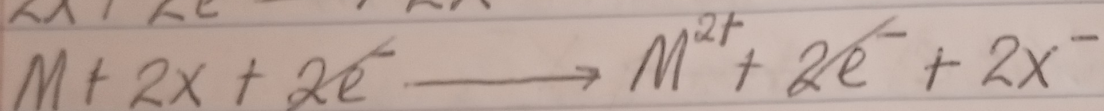
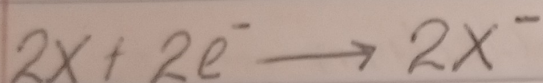
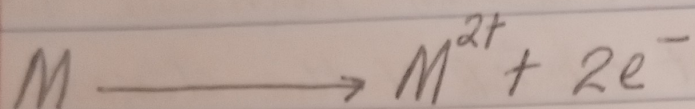
Because hydrogen can release its electron to form a bonding

HCl NaCl KCl : Similar because they are

in group one.



This is a 1:1 ratio



Formula use to determine the force of attraction

$$F_a = \frac{Z^+ X^- e^2}{4\pi\epsilon_0 r^2}$$

e is the charge $= 1.602 \times 10^{-19}$

Repulsive energy is given by E_r

$$E_r = \frac{B}{r^n}$$

r^* = radius

n = number of shells

B = Constant of proportionality

When you add the repulsive and the force of attraction, a bond is obtained.

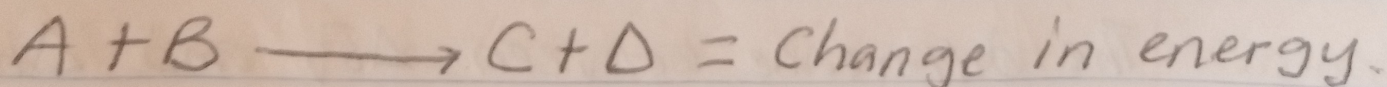
$$E_c = \frac{Z^+ X^- e^2}{4\pi\epsilon_0 r} + \frac{B}{r^n}$$

Ionic bonding is the strongest bond but not only the strongest bond.

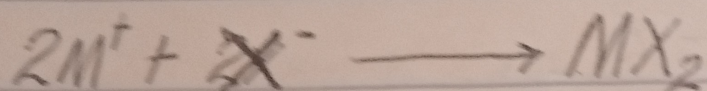
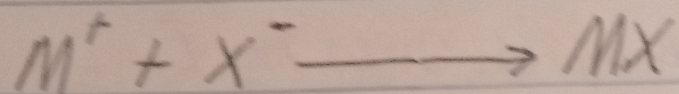
5th September, 2023

BORN-HABER CYCLE AND THERMOCHEMICAL ~~AND~~ CALCULATION

If you know the reactants and you get the products, you can be able to calculate the energy



The lattice energy of an ionic crystal is equivalent to its heat of formation of 1 mole of its ionic constituents in the gas phase.



The heat of formation can be determined experimentally.

- By the use of instruments
- By thermochemical calculations.

HEAT OF FORMATION

It is the thermal effect of a reaction associated with the formation of 1 mole of substance from its constituent

This could be by change in Internal energy, E of the system or Enthalpy, H .

INTERNAL ENERGY CHANGE ΔE_v

Is the energy effect at constant volume

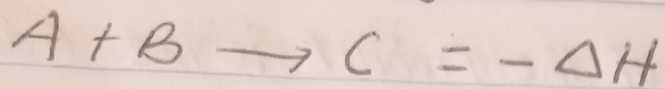
ENTHALPY CHANGE ΔH_p

Is the energy effect at constant pressure.

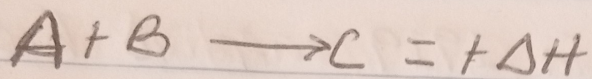
The difference between ΔE_v and ΔH_p is $P\Delta V$

$$\Delta H = \Delta E + P\Delta V$$

Exothermic rxn is obtained when heat is given out of the surrounding.



Endothermic rxn is obtained when heat is absorbed by the system.



The Equations of chemical reaction of

- It is also indicate the States of the reacting species are given in a thermochemical equation.
- They are done at standard temperature and Pressure

Standard temperature could be $^{\circ}\text{C}$ or Kelvin.
 25°C

Standard Pressure could be in mmHg or Pa i.e
760 mmHg or $1.01325 \times 10^5 \text{ Pa}$

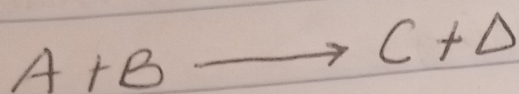
Therefore, standard effect are designated as E
These are based on Hess's law

Hess's law states that the enthalpy of a reaction is given irrespective of the number of intermediate

Examinable

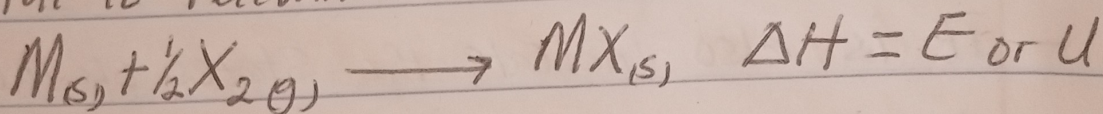
Steps involved in going to the product.

Mechanism is the step involved

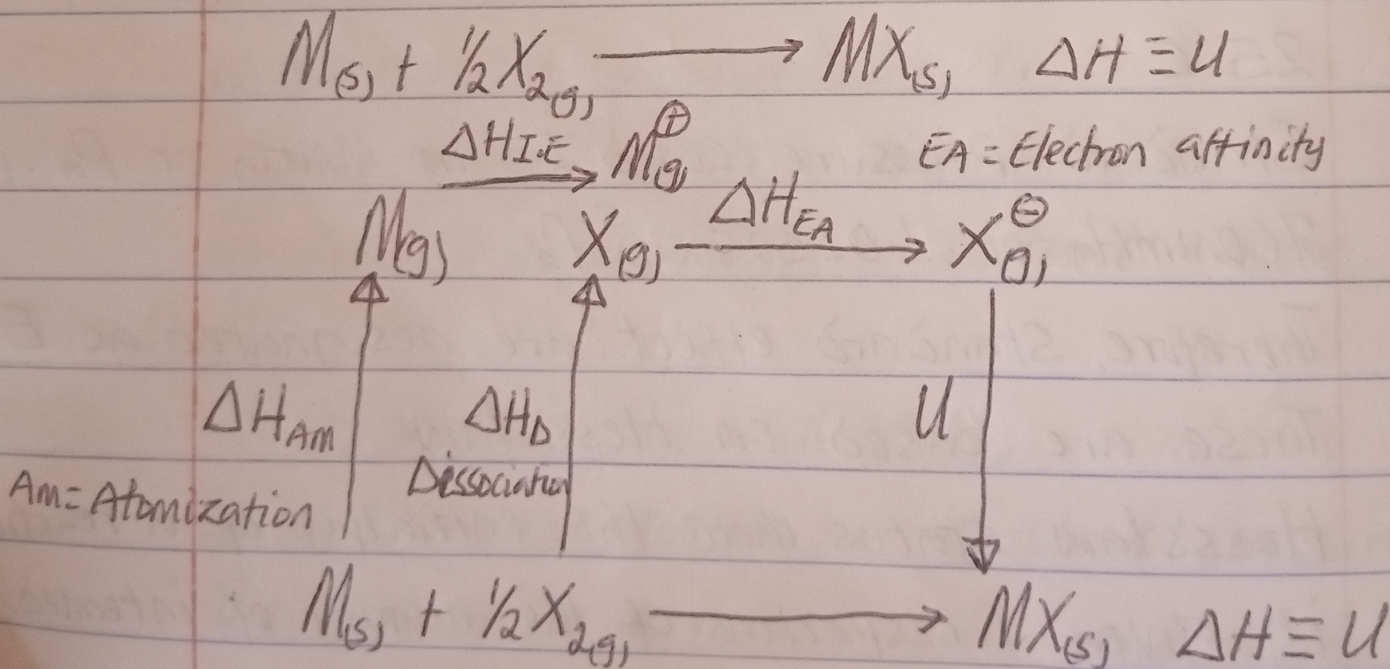


Formation of the product is the addition of the heat of formation of A - the heat of formation of B

Born-Haber in 1919 applied his law to ionic crystals; and is related to lattice energy of the crystal to relevance thermochemical equation.



The lattice energy of the above rxn cannot be experimentally determined.



$$\Delta H_f = \Delta H_{Am} + \Delta H_{I.E} + \frac{1}{2} \Delta H_D + \Delta H_{EA} + U$$

Example 1: What is the change in internal energy for the formation of NaCl if the following are given

$$\Delta H_{Am} = 107.3 \text{ KJmol}^{-1}$$

$$\Delta H_{I.E} = 495.8 \text{ KJmol}^{-1}$$

$$\Delta H_D = 122 \text{ KJmol}^{-1}$$

$$\Delta H_{EA} = -348.6 \text{ KJmol}^{-1}$$

$$U = 787 \text{ KJmol}^{-1}$$

Born-Haber Cycle is the application of his law to obtain ionic crystals of thermochemical equation.

COORDINATION NUMBER (CN)

According to Pauling 1st rule says when a coordination polyhedron is formed around each cation, the distance between the cation and the anion can be determined by the sum of the radii.

The coordination number of the cation can be determined by the ratio of the cation.

The Coordination number: Is equal to the number of cation or ions of X which surrounds a central atom or metal ion. CN is the function of the difference in

Sizes of N. The $\propto$ the difference the smaller the Coordination number and vice versa.

They are determined by Pauling 2nd rule in a Perfect Crystal

Pauling 2nd rule states that the valency of an ~~stable~~ anion in a stable ionic structure tends to compensate the strength of electrostatic bond which reach it from the cation situated at the ^{Centre} of the Polyhedron of which the anion is at the vertex and vice versa.

This means that the charge of an particular ion e.g anion must be balance. To estimate the amount of effective charge, it must be given a charge M_i and the coordination number CN_i and the electrostatic bond strength S_i is the ratio of the charge number to the coordination number in an ionic crystal.

$$S_i = \frac{M_i}{CN_i}$$

$$S_i = X$$

$$\text{Where } X = \sum_{i=1}^n \frac{M_i}{CN_i}$$

Example 2: Calculate the electrostatic bond strength of Sodium chloride, $\text{NaCl} \rightleftharpoons \text{Na}^+ \text{Cl}^-$.
Sodium, Na^+ has 6 ions, 6 Cl^-

Solution

$$S_i = \frac{1}{6}$$

$$X = \sum_{i=1}^n \left(\frac{1}{6}\right) = 1 \quad \text{i.e.} \quad \frac{\frac{1}{6}}{\frac{1}{6}} = \frac{1}{6} \times \frac{6}{1} = \frac{6}{6} = 1 = \underline{\underline{1}}$$

2. Calculate the S_i for Titanium Oxide TiO_2 with rutile structure of Ti^{4+} surrounded by 6 O^{2-}

Solution

$$\text{This implies that } S_i = \frac{4}{6} = \frac{2}{3}$$

$$X = \sum_{i=1}^3 S_i = \sum_{i=1}^3 \frac{2}{3} = 3\left(\frac{2}{3}\right) = \frac{3 \times 2}{3} = \frac{6}{3} = \underline{\underline{2}}$$

IONIC BONDING

- i Properties of Ionic compounds
- ii Factors affecting the formation of compounds.
- iii. Ionic crystals Structure
- iv. Building of ionic crystal
- v. Types of unit cells
- vi Shape of unit cells

Vii. Structure of simple ionic solids.

Properties of Ionic Compounds

1. Ionic compounds have melting and boiling points. Due to the electrostatic force binding the ions. Ionic states; Solid, liquid and gas.
2. Electrical conductivity: Ionic solids do not conduct electricity but in molten state. This is because ions are tightly bonded and does not move freely while the molten or solution form moves freely.
3. Solubility: They are soluble in polar solvents. The polar solvents includes; Water, ethanol, Esters, Aldehydes etc but are not soluble in non-polar solvents.

The formula calculating

$$E = \frac{q_1 q_2}{4\pi r^2 \epsilon_0}$$

Where E = Energy, $q_1 q_2$ = Two charges.

r = Distance separating the ions

ϵ_0 = Permittivity of free space

4. Hardness and brittleness: Ionic solids are hard and brittle. The electrostatic bond binding the elements together makes it hard. The energy required to break the binding forces between atoms makes it strong.

Factors affecting the formation of Ionic Compounds

1. Formation of Positive ions M^+
2. Formation of negative ions X^-
3. Stable ionic compounds which has to do with lattice energy $U = H_f$

Lattice energy is the energy required to break two or more binding atoms to separate ways.

1. Ionization energy
2. Electron affinity
3. Lattice energy

Ionic Crystals Structure

- In ionic solid, ions of Positive charges are present and the negative charges must be present.
- The positive and negative charges must be balanced
- For every species formed they must be cancellation of repulsive and attractive form.

Building of Ionic crystals

Kossel (1916)

Charge ions are regarded as rigid sphere. The structure of the size of the binding atoms.

Examinable

Show that Coulombic force is giving by

effective

$$F = \frac{e_1 e_2}{(r_1 + r_2)^2} \cdot \frac{1}{\epsilon_0}$$

nuclear is

inversely e_1, e_2 = Respective charges of two elements.

proportional r_1, r_2 = Ionic radii

to the Coulombic ϵ_0 = Permittivity of free space = $8.854 \times 10^{-12} \text{ Fm}^{-1}$

force. F = force (Coulombic force)

$$F \propto \frac{1}{Z^*} \quad [\text{Pauling rule}]$$

Where Z^* = Effective nuclear charge

$$r_{M^+} \propto \frac{1}{Z_{M^+}^*} = \frac{K}{Z_{M^+}^*} \quad \text{--- (1)}$$

$$r_{X^-} \propto \frac{1}{Z_{X^-}^*} = \frac{K}{Z_{X^-}^*} \quad \text{--- (2)}$$

Dividing equation (1) and (2)

$$\frac{K}{Z_{X^-}^*} \cdot \frac{r_{M^+}}{r_{X^-}} = \frac{K}{\frac{Z_{M^+}^*}{\frac{K}{Z_{X^-}^*}}}$$

Starting

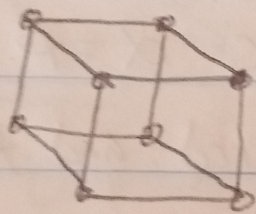
1. Ions [Positive and negative]

Angle, length and name of the shape.

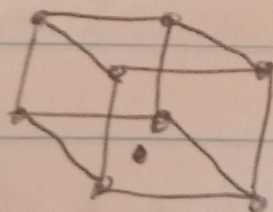
- This spatial order of ~~atom~~ is called Crystal Structure.
- The basic building block is called the unit cell and is defined as the smallest grouping that repeats itself over and over again in space to give the full symmetry of the crystal structure. In ionic solids the building blocks are electrically charged particles (cations and anions) in a three dimensional form (3D).
- Lattice is the arrangement of positive and negative ions repeatedly in an array. This array is called Point Lattice. Each lattice point has identical environment.

Types of unit cells

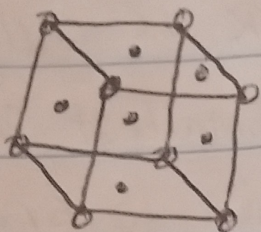
1. Primitive unit cell: P. It has the smallest point lattice at the corners of the



2. Body Centered unit cell, I.

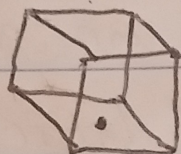
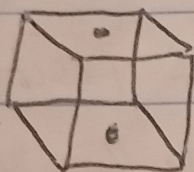


3. Face - Centered unit cell



For each cell  there is dot in the middle 

4. Based centered, C.



Shapes of unit cells

There are Seven (7) unit cell shapes viz:

1. Cubic $a = b = c$ $\alpha = \beta = \gamma = 90^\circ$

Primitive, Body centered, and Face centered

P, I, F

2. Tetragonal

3. Hexagonal

4. Orthorhombic

5. Triclinic

6. Rhombohedral

1. Density (Mass/volume) of the ionic crystals Structure

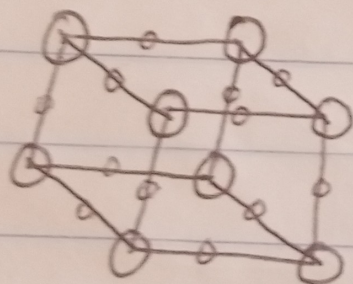
They are Six (6) Structure of Simple ionic Solids.

1. Rock or NaCl Structure / CaO , MnO , CaS
2. Caesium Chloride Structure / CsCl , TlCl
3. Zinc blende Structure / CuSO_4 , CuS
4. Zinc oxide Structure / BeO
5. Calcium fluoride Structure / NH_4F
6. Rutile Structure / TiO_2

THE SODIUM STRUCTURE

$\bigcirc \text{Na}^+$

$\bigcirc \text{Cl}^-$



The ratio is 1:1

POLARIZATION AND PARTIAL COVALENCY IN IONIC SOLID.

Polarization is a process by which ^{bonding} the complete formation due to the delocalization of electrons.

Polarizable: having the tendency to Polarization.
Polarization is

Effects of Polarizations in Ionic Solids

There are five (5) effects of Polarization in ionic solids.

1. Variation of inter-atomic distance falls as the Polarization increases.
2. Abnormally large value of lattice energy, U .
3. Reduction in coordination number
4. Lowers the melting point in ionic crystals.
5. A more Polarized compound will be less Soluble in Polar solvents.

Factors affecting Polarization in Ionic Solids